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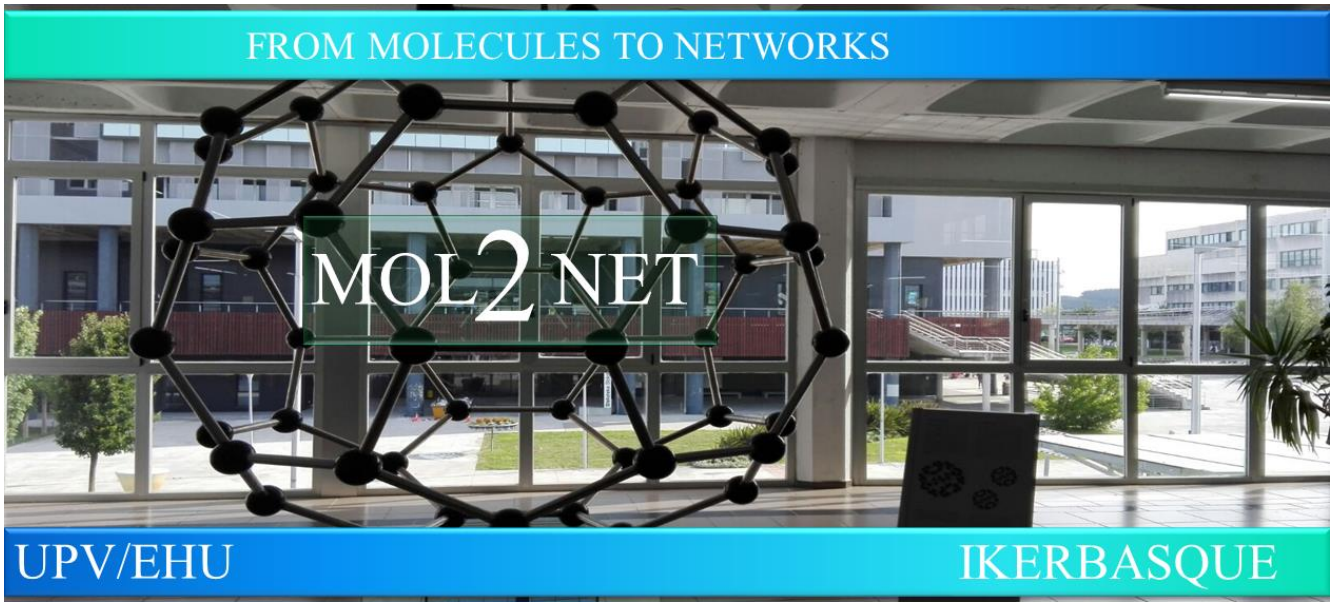
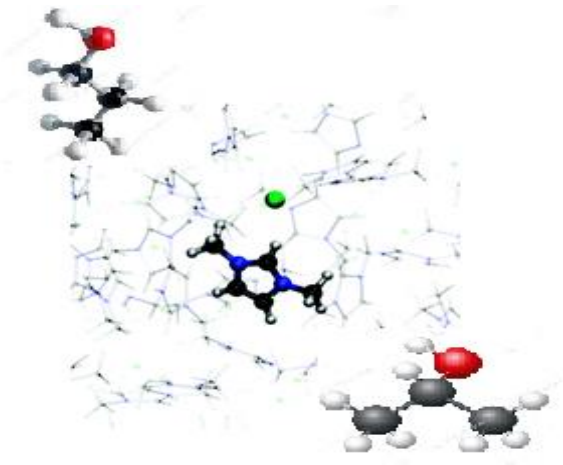


Dynamic inhomogeneity in highly diluted solutions of ionic liquids with isomers of monohydric alcohols

N.Atamas[a], I. Matushko[a], G.Taranyik[b]
[a] National Taras Schevchenko University of Kyiv, 6a Gluschkov Ave., Kyiv, Ukraine
[b]International European University, Kyiv, Ukraine

Graphical Abstract



Abstract.
During the study, the influence of the isomerism of monohydric alcohols on their time dynamics in an ionic liquid was studied. Based on the data obtained as a result of molecular dynamics calculations, the time intervals were determined during which the nature of the motion of a dissolved substance (iso-alcohol molecules) in an ionic liquid changes, model representations were constructed to describe the mechanisms of diffusion of the components of the systems under study, which made it possible to analyze the effect of isomerism of monatomic alcohols on the dynamic properties of alcohols in an ionic liquid.

Introduction

Ionic liquids (ILs) attract more and more scientific research due to their unique physicochemical properties, such as non-volatility, high thermal stability, high ionic conductivity, wide electrochemical windows, and excellent solubility in many organic and inorganic substances. ILs are often used as a medium for green solvent extraction processes, as a recyclable alternative to organic solvents, as catalysts for organic synthesis, as environmentally friendly solvents, and as media for analytical and physical chemistry. For technological purposes, ILs are rarely used in their pure form: they will almost always be diluted either with reagents and products, or with the presence of a co-solvent specially added to optimize the physicochemical characteristics of the IL-systems.

Materials and Methods

To conduct a computer-based experiment the molecular dynamics method in the modified DL_POLY_4.05 [1] software package with a time step of 2 fs will be used. In the calculations, cations, and anions of IL, and dissolved molecules will be represented as the rigid charged models with a fixed geometry. To describe interactions between ions at short distances in an ionic liquid, the Buckingham potential will be used. The effective intermolecular interaction potential, which can be represented as the sum of the Lennard-Jones and Coulomb components, both describe the interactions between the components of the ionic liquid at large distances, describe the interactions between the components of the IL and the dissolved substance. The Berenzen thermostat will be used to stabilize the system in the NVT ensemble. In the calculations, the electrostatic interaction at short distances will be modeled by placing point charges on each atom, and long-range electrostatic interaction will be modeled using summation by the Ewald method. To determine the energy characteristics, several series of independent calculations will be carried out with steps of 200 fs, 160 fs, and 80 fs. Calculations will be performed as follows: the system investigated was stabilized in 8×10^5 steps, followed by another 15×10^5 steps of calculation. All radial distribution functions (RDFs) will be obtained with a step of ~200 fs.

Results and Discussion

According to previous studies [2-4]: “When an alcohol molecule is dissolved in dimethylimidazolium chloride $dmim^+/Cl$-, the local structure of the IL changes, and it can form hydrogen bonds with the $dmim^+/Cl–$ components. The existing local structure can act as “defects” leading to a slow different diffusion regime of all components in the $dmim^+/Cl^–$ – alcohol system. In other words, they confirm the assumption about the heterogeneity of the dynamics of the components of the $dmim^+/Cl^–$ – alcohol system.” Therefore, the dissolution of monoalcohols and iso-monoalcohols in IL solutions should lead to similar processes.

Conclusions

As part of the research, the following tasks were solved:

1. Correction and further development of the methodology for determining the intervals for changing modes of motion in liquids, proposed in [3,4], the construction of model representations for diffusion mechanisms at different time intervals.
2. As part of the study, the influence of the structure of alcohols (propanol) and isomonoalcohols (isopropanol) on the dynamic inhomogeneity of the movement of components of systems based on ionic liquids was studied, which will make it possible to obtain information about the mechanisms of diffusion in the systems under study at the microlevel.

References

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